Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic Supporting Information

Enhanced catalytic activity and near room temperature gas sensing properties of SnO_2 nanoclusters@mesoporous Sn(IV) organophosphonate composite

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Table S1: Solvent optimization for deoximation reaction catalyzed by **SnO_2@MSnP**.

Sl. No.	Solvent	Catalyst Amount (wt%)	% Yield
1	CH_3COCH_3:H_2O (1:1)	10	96
2	CH_3CN	10	21
3	C_2H_5OH	10	10
4	CH_3COCH_3	10	~0
5	H_2O	10	~0

Table S2: Amount of catalyst optimization for deoximation reaction catalyzed by **SnO_2@MSnP**.

Sl. No	Solvent	Catalyst Amount (wt%)	% Yield
1	CH_3COCH_3:H_2O (1:1)	1.7	50
2	CH_3COCH_3:H_2O (1:1)	3.3	65
3	CH_3COCH_3:H_2O (1:1)	6.7	75
4	CH_3COCH_3:H_2O (1:1)	10	96

Table S3: Activity comparison with different catalysts taking acetophenone oxime as substrate

Sl. No.	Name	Catalyst Amount (wt %)	% Yield
1	None	-	~0
2	Mesityl-1,3,5-tris (methylenephosphonic acid)	10	100
3	$SnCl_4.5H_2O$	10	99
4	SnO_2	10	55
5	Sn(IV)phenyl phosphonate	10	5
7	SnO_2@MSnP	10	96

Table S4: SnO_2 as catalyst for esterification of free fatty acid.

Reaction Time (h)	Temperature ˚C	Methanol :oil ratio	Catalyst used (wt%)	Conversion (%)
0	60	6:1	2	~0
1	60	6:1	2	9.8
2	60	6:1	2	20.8
3	60	6:1	2	42.9

Table S5: **SnO_2@MSnP** as catalyst for esterification of free fatty acid.

Reaction Time (h)	Temperature ˚C	Methanol :oil ratio	Catalyst used (wt%)	Free fatty acid content (mg KOH/gm of oil)
0	60	6:1	2	~0
1	60	6:1	2	36.1
2	60	6:1	2	70.7
3	60	6:1	2	88.6

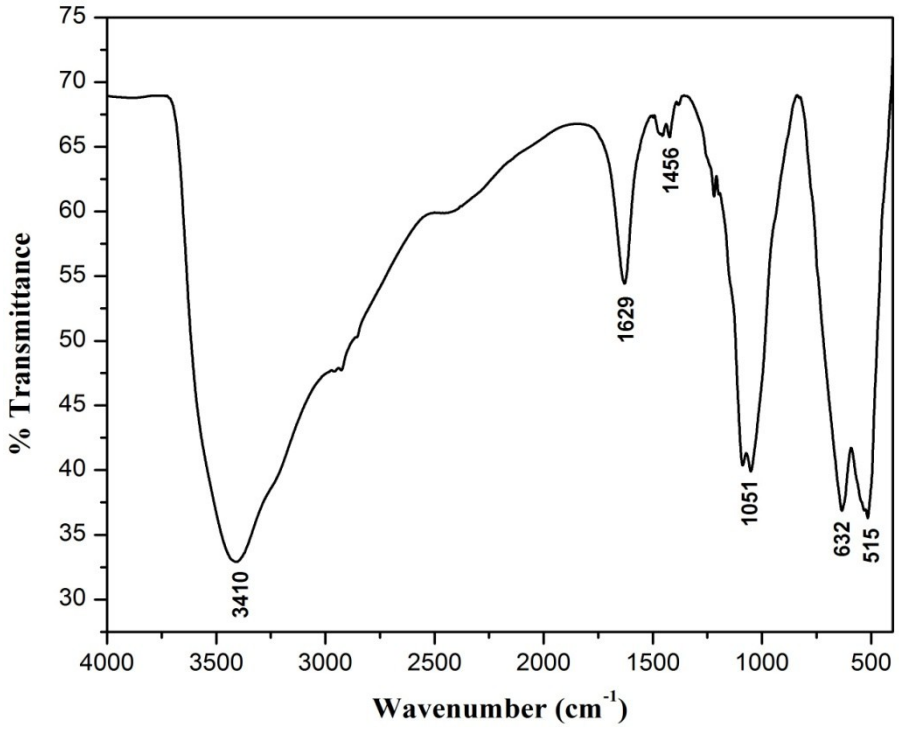


Figure S1: FT-IR spectrum of **SnO_2@MSnP** as KBr disc.

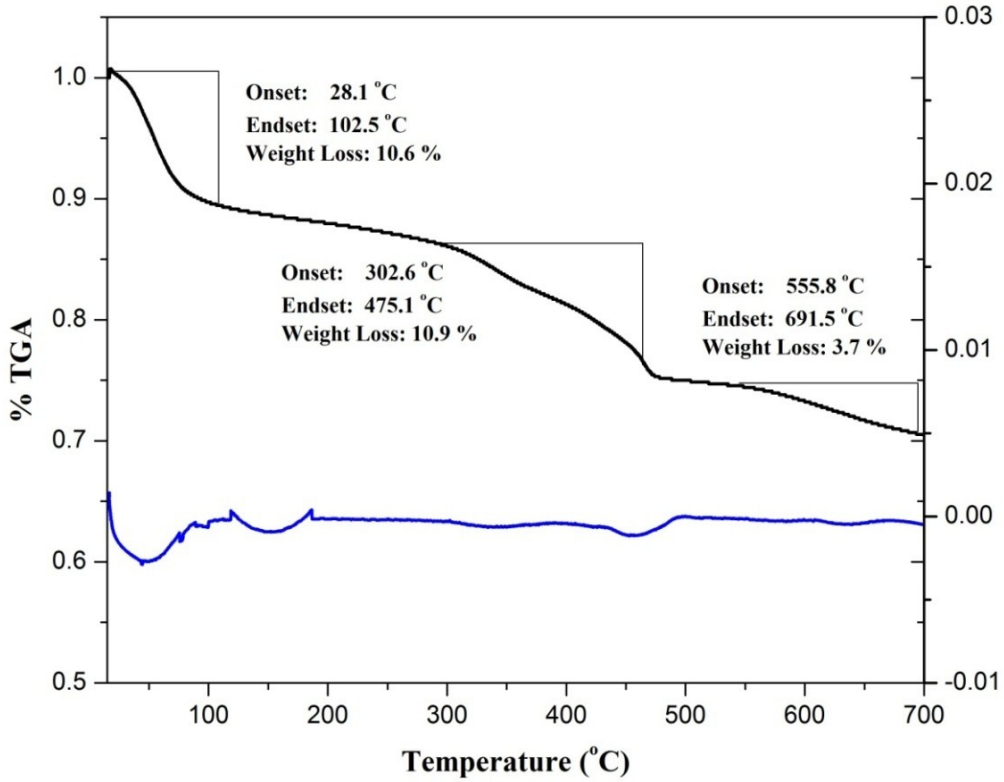


Figure S2: Thermogravimetric analysis spectrum of **SnO_2@MSnP**.

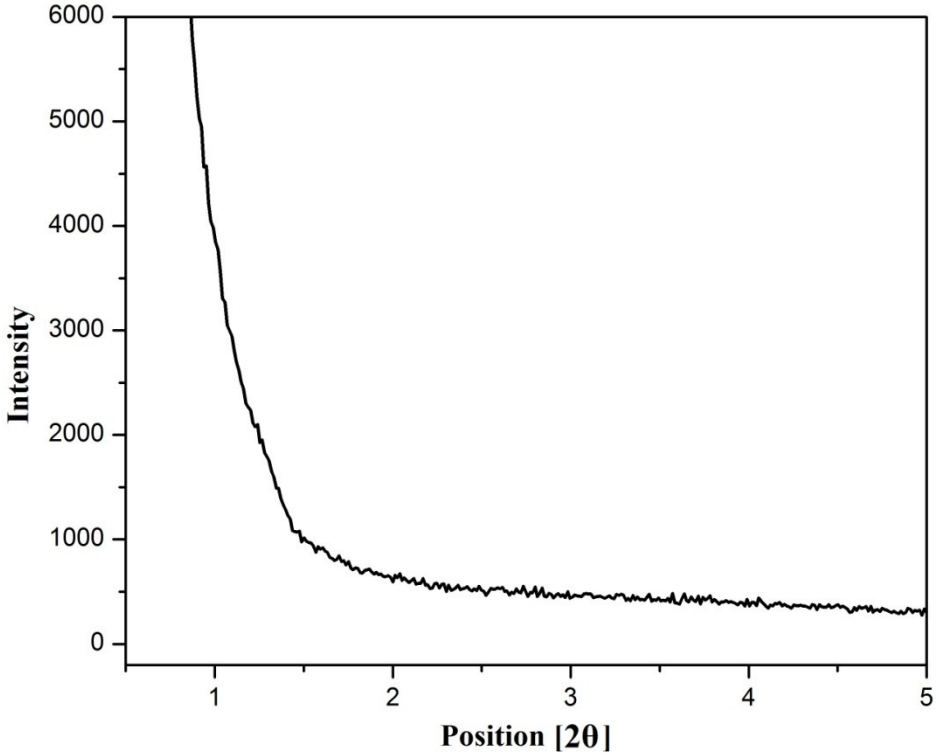
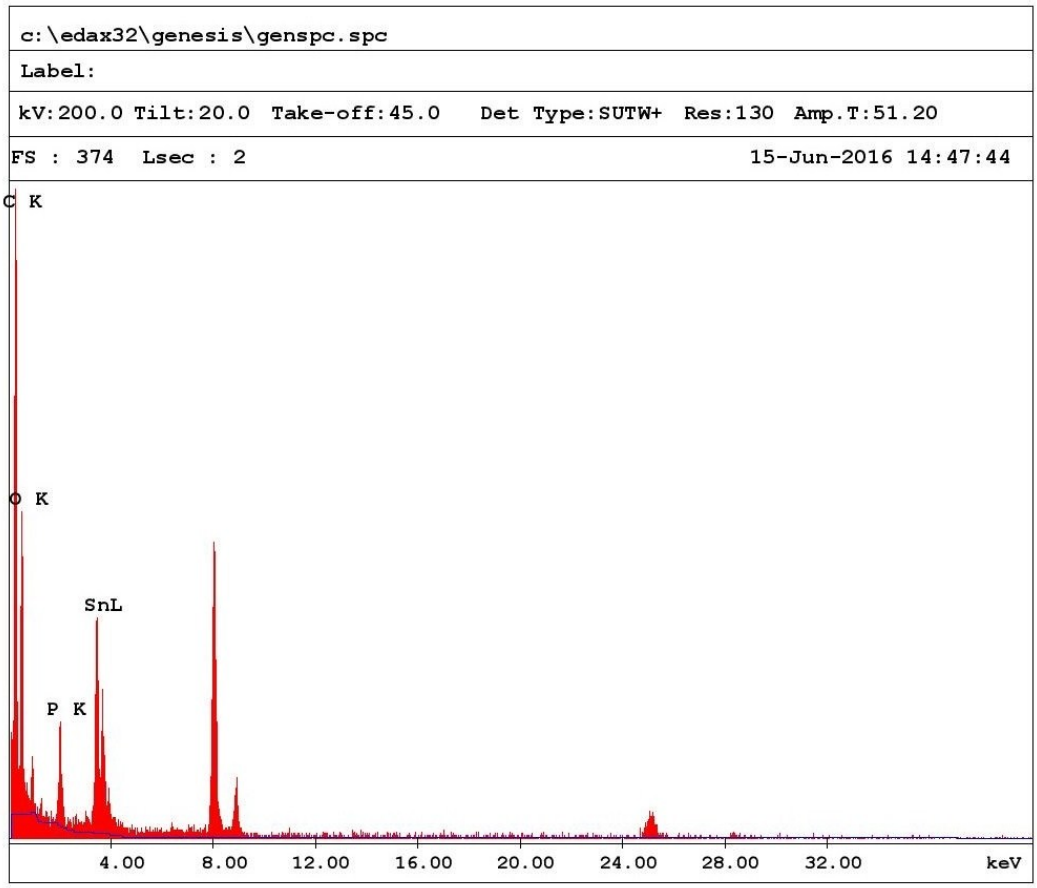


Figure S3: Small angle powder XRD spectrum of SnO_2@MSnP.



EDAX ZAF Quantification (Standardless)
Element Normalized
SEC Table : Default

Element	Wt %	At %	K-Ratio	Z	A	F
C K	65.57	72.58	0.3846	1.0034	0.5843	1.0005
O K	32.48	26.99	0.0461	0.9978	0.1423	1.0000
P K	0.67	0.29	0.0040	0.9555	0.6161	1.0017
SnL	1.28	0.14	0.0342	0.8703	3.0559	1.0000
Total	100.00	100.00				

Element	Net Inte.	Bkgd Inte.	Inte. Error	P/B
C K	860.63	36.59	2.34	23.52
O K	363.68	36.59	3.79	9.94
P K	185.98	29.18	5.55	6.37
SnL	492.60	14.37	3.06	34.27

Figure S4: TEM-EDX image of **SnO_2@MSnP**.

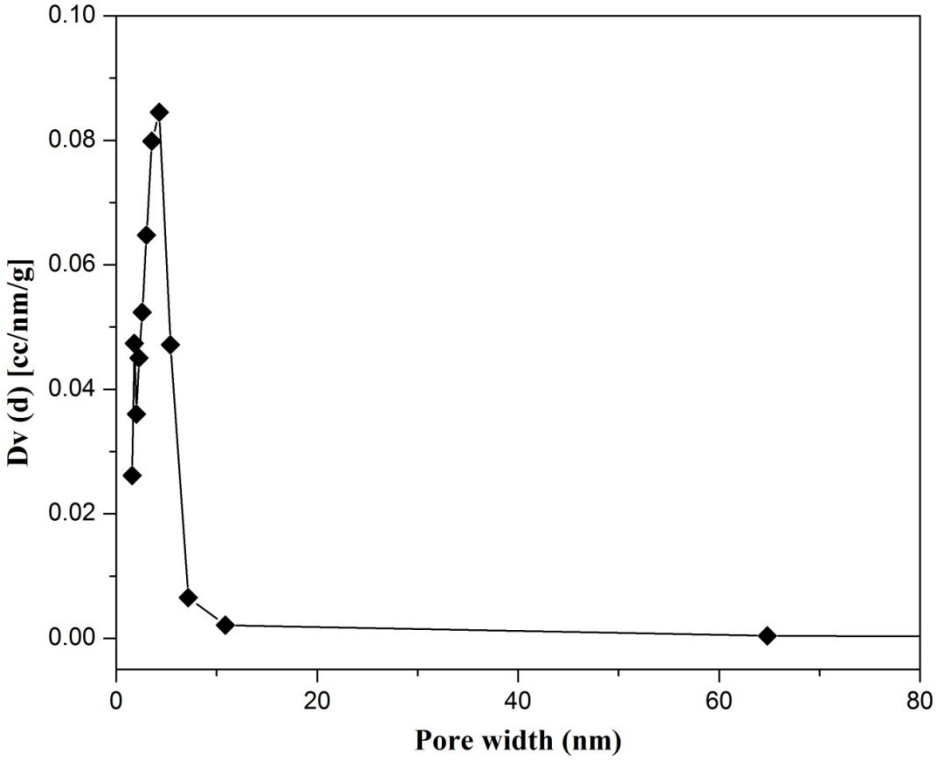


Figure S5: BJH pore size distribution of **SnO_2@MSnP**.

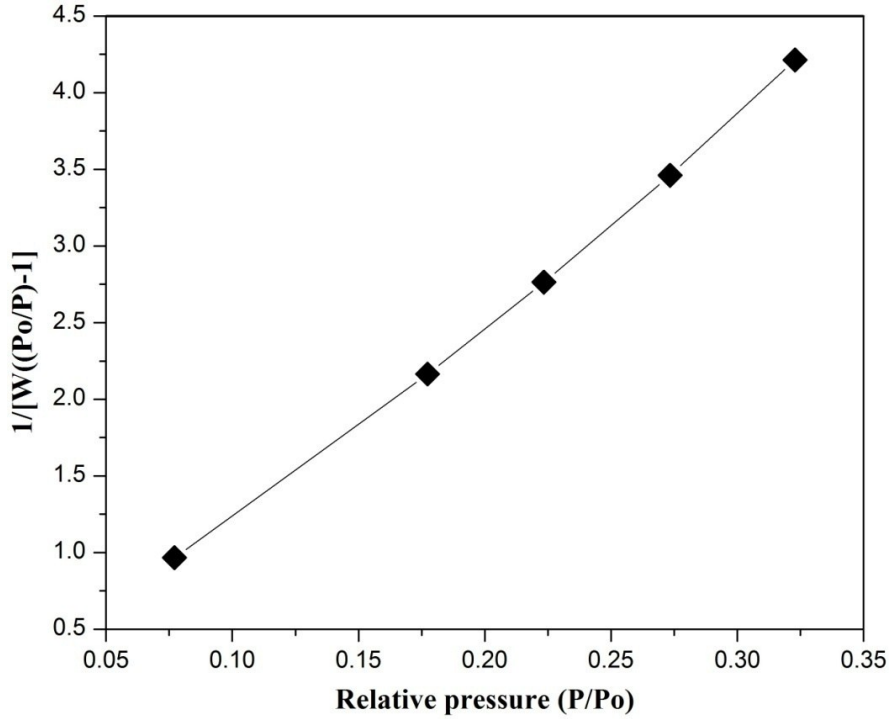


Figure S6: Surface area analysis plot of **SnO_2@MSnP**.

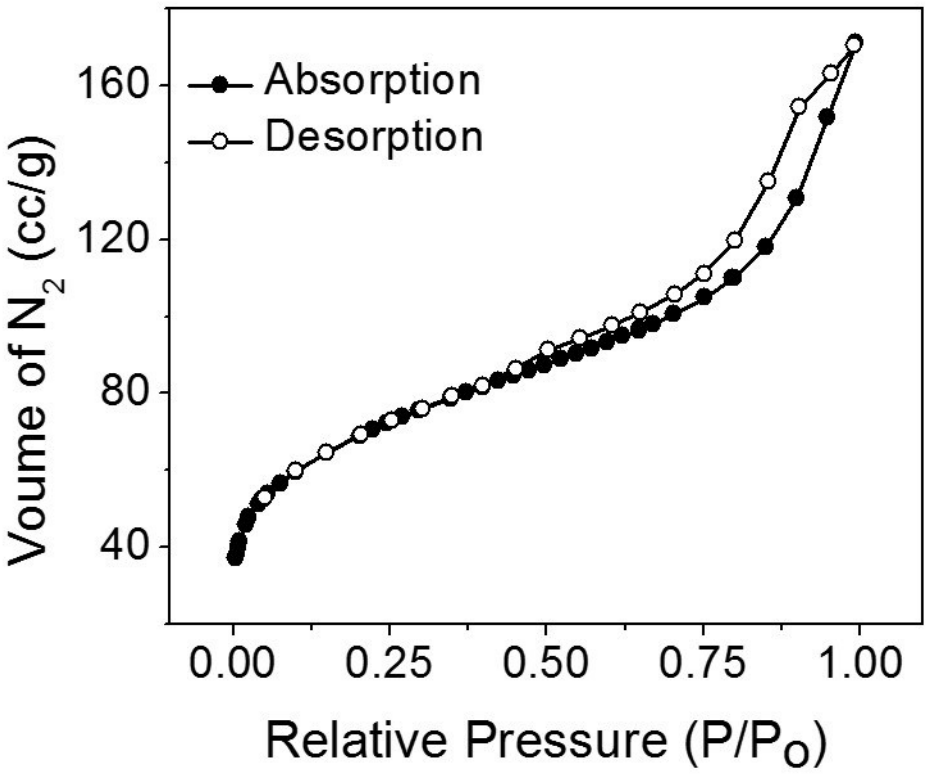


Figure S7: The BET surface area of pristine SnO_2 nanoparticles

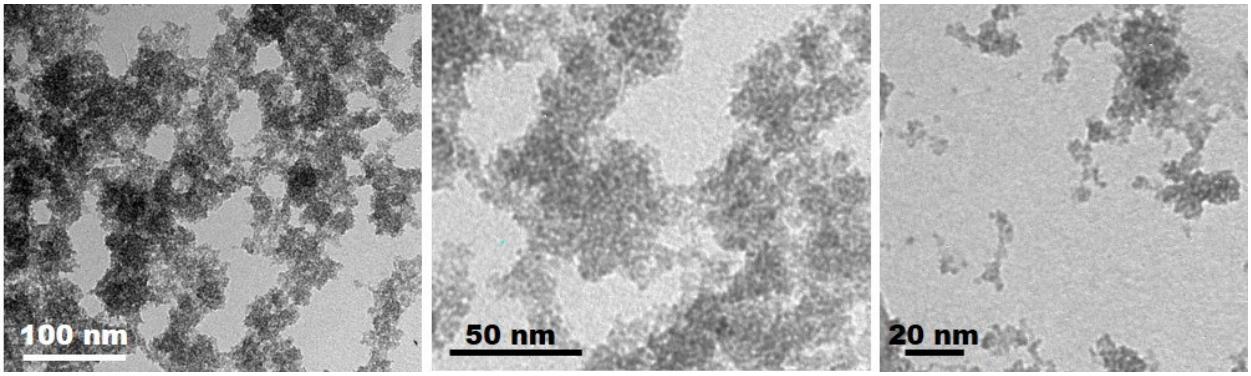


Figure S8: TEM images of pristine SnO_2 nanoparticles

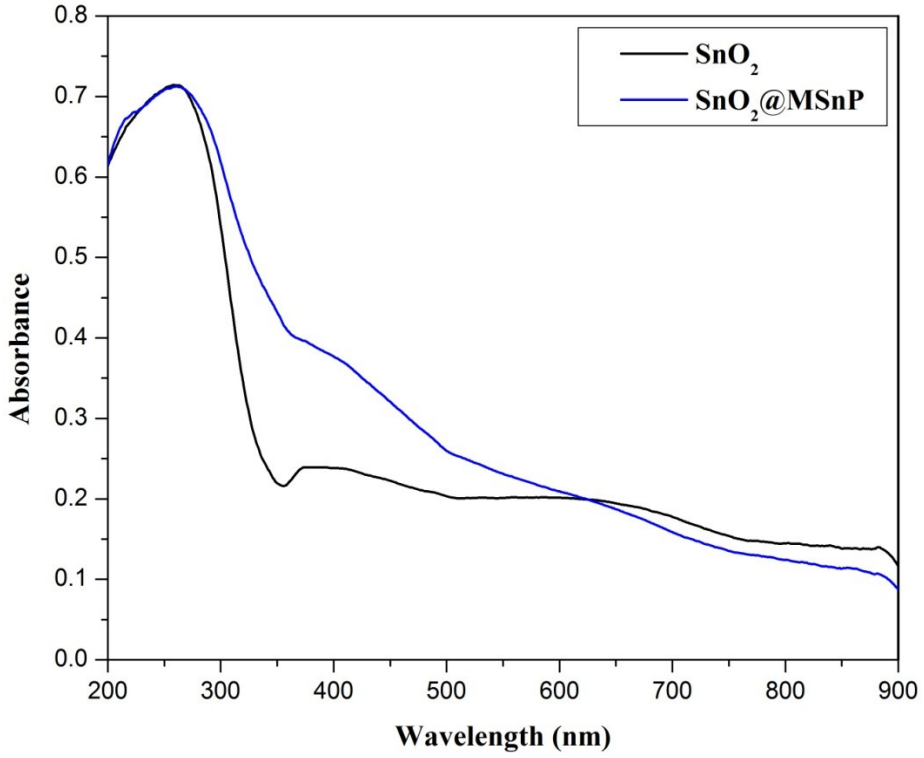


Figure S9: UV-visible spectrum of **SnO_2** and **SnO_2@MSnP**.

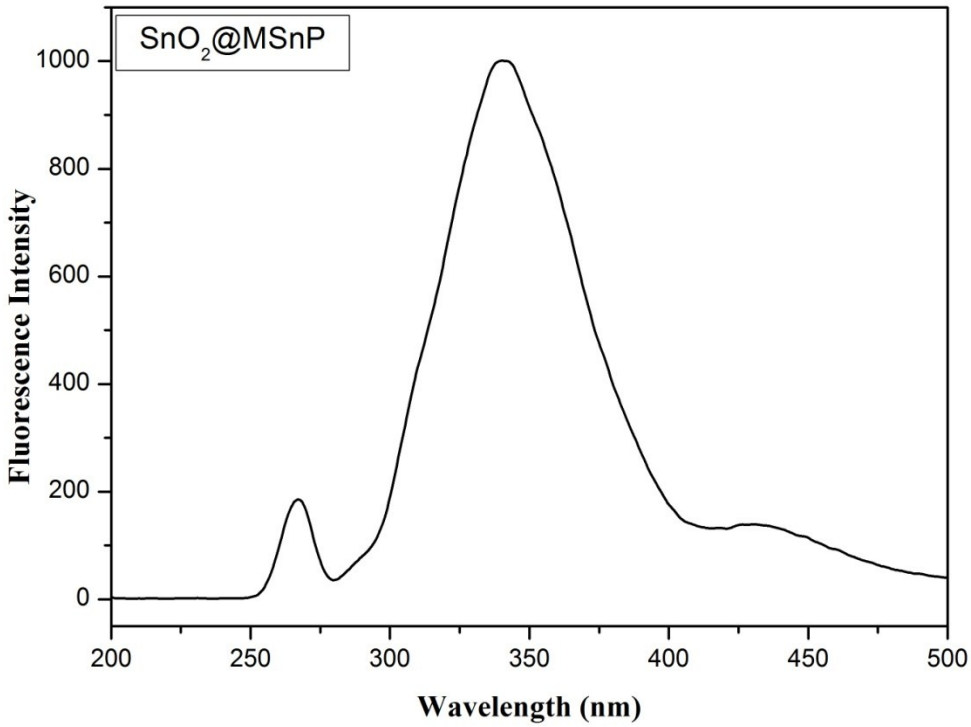


Figure S10: Fluorescence spectrum of **SnO_2@MSnP**.

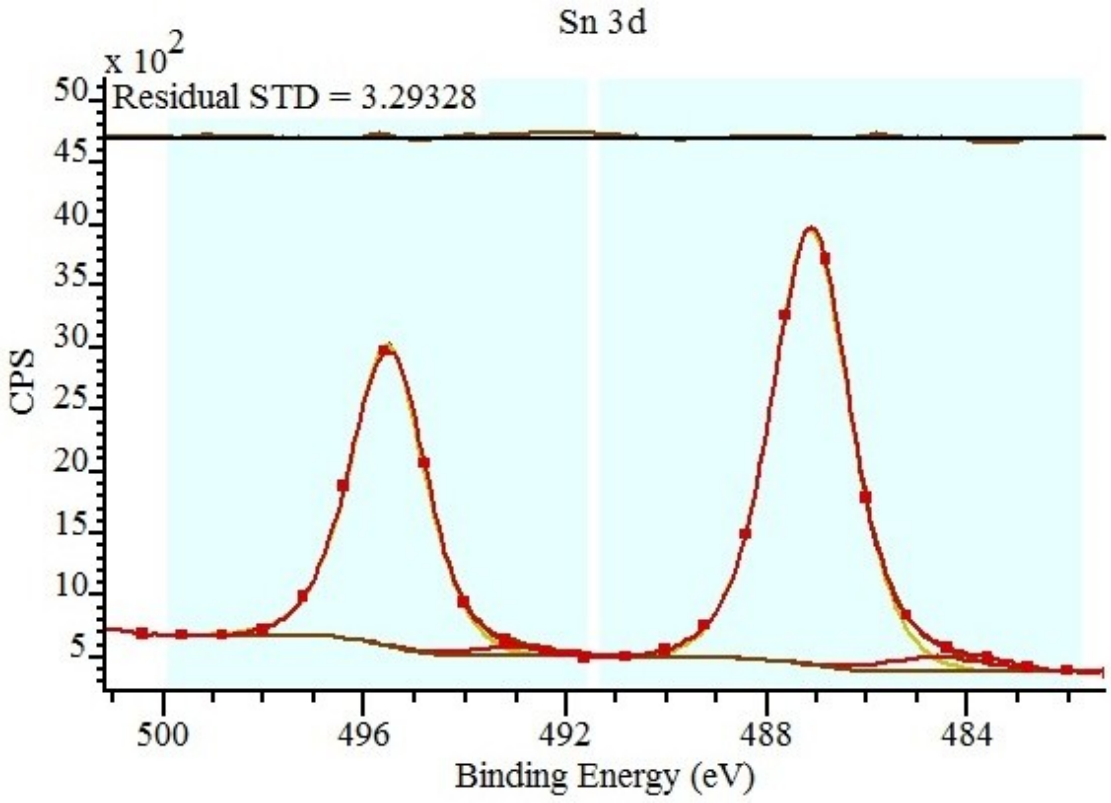


Figure S11: The XPS spectra of Sn 3d regions of **SnO_2@MSnP**.

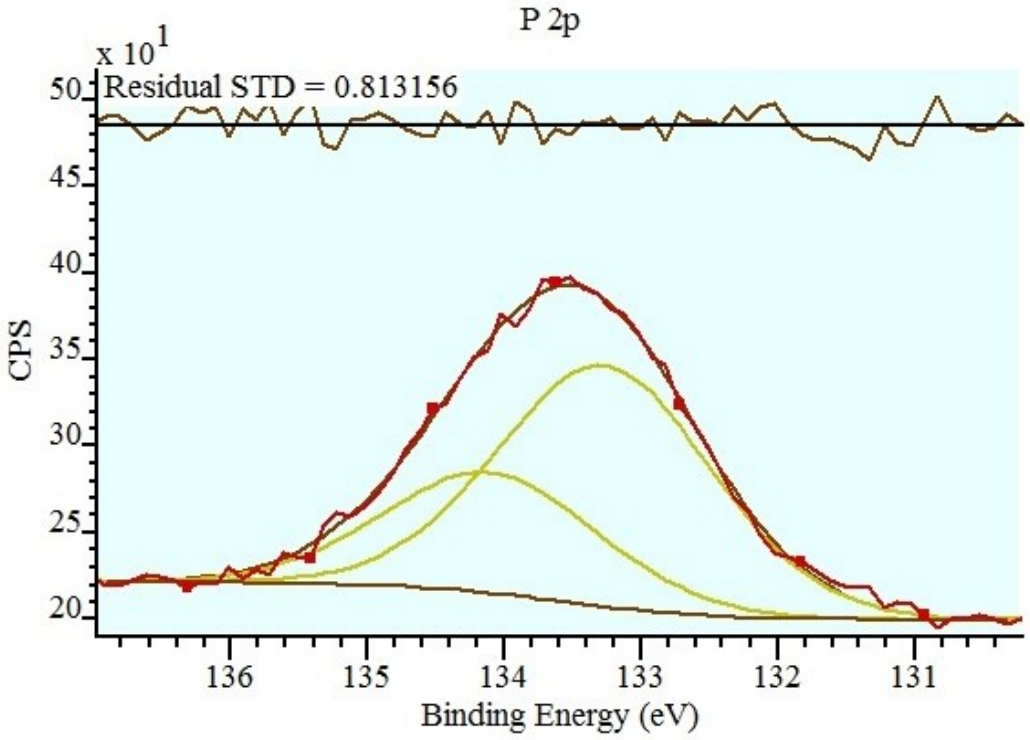


Figure S12: The XPS spectra of P 2p regions of **SnO_2@MSnP**.

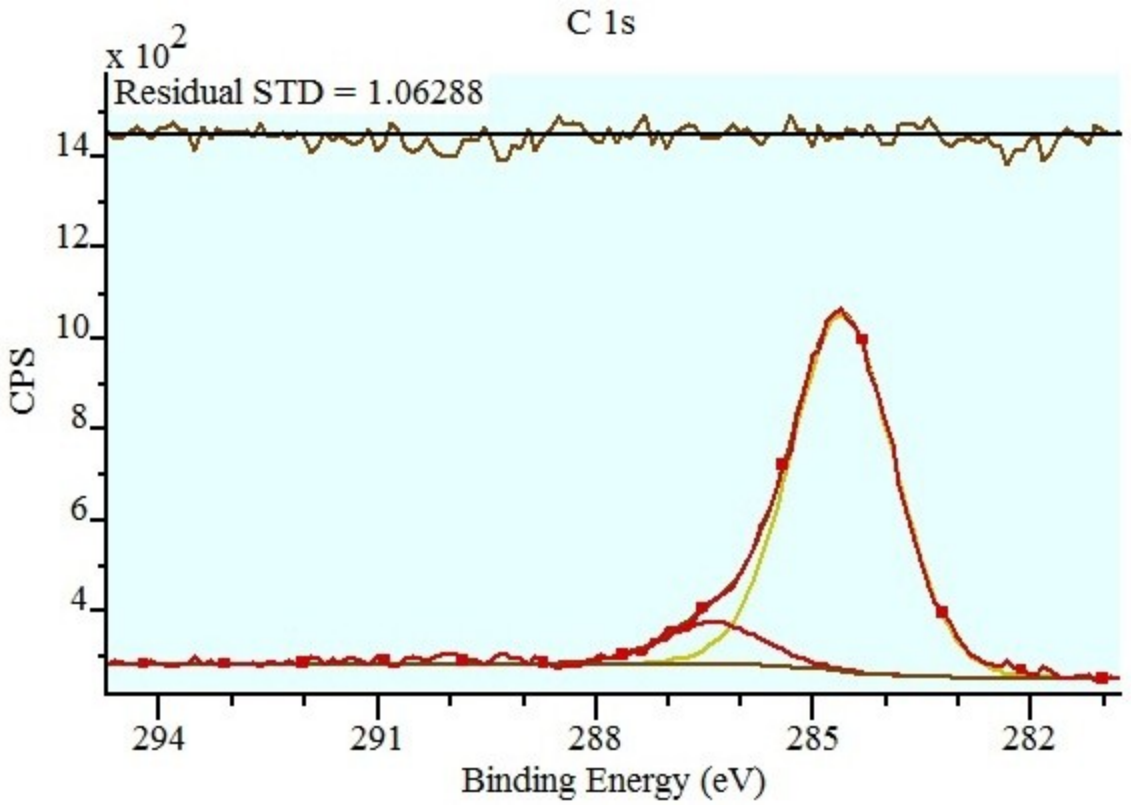


Figure S13: The XPS spectra of C 1s regions of **SnO_2@MSnP**.

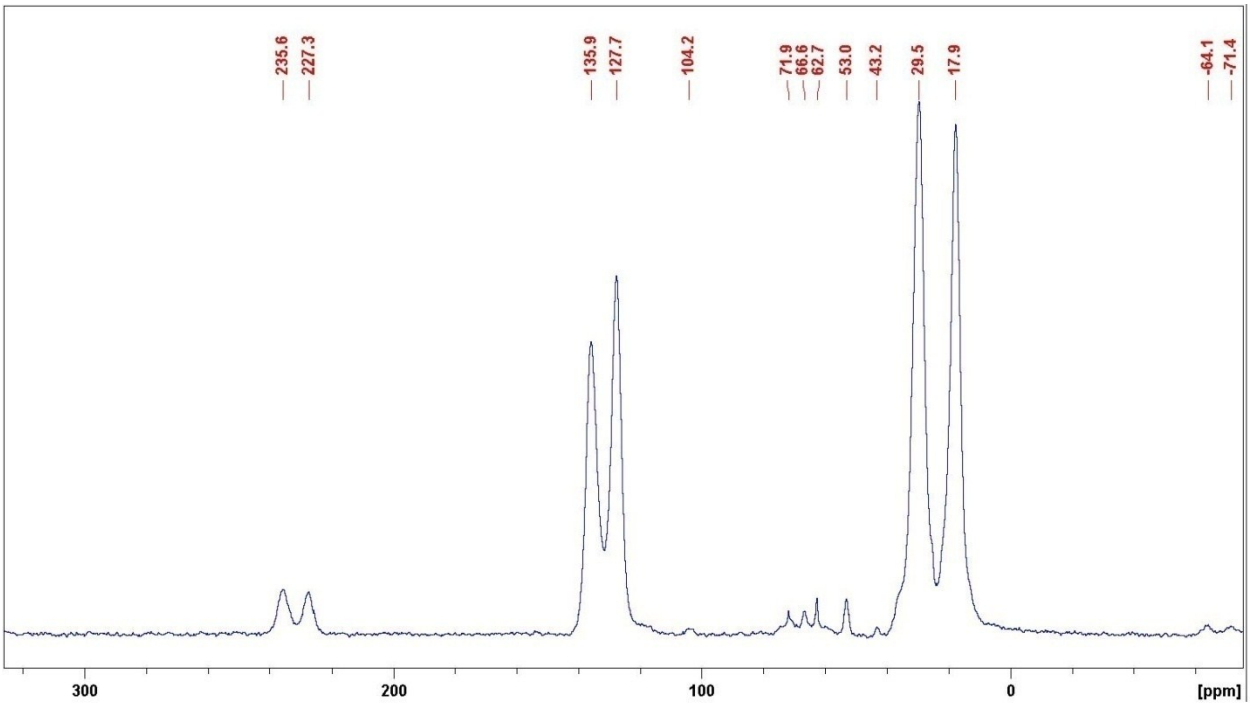


Figure S14: ^{13}C MAS 12.5 KHz NMR spectrum of **SnO_2@MSnP**.

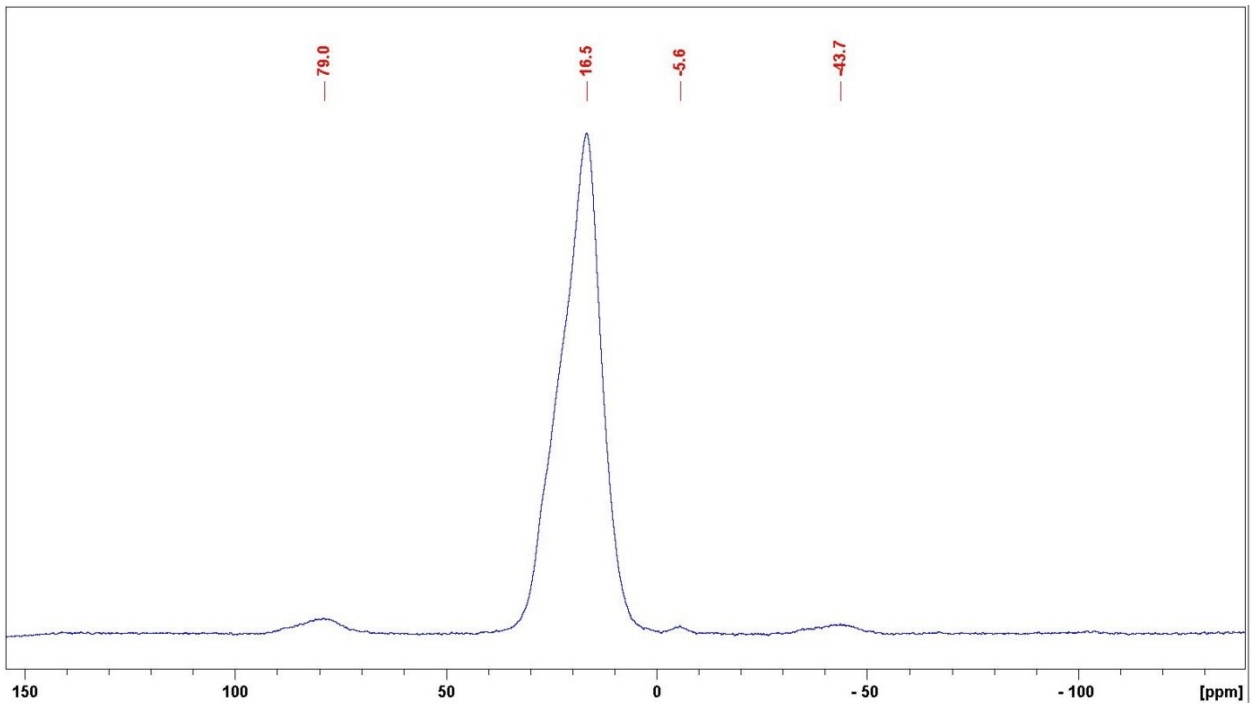


Figure S15: ^{31}P MAS 12.5 KHz NMR spectrum of **SnO_2@MSnP**.

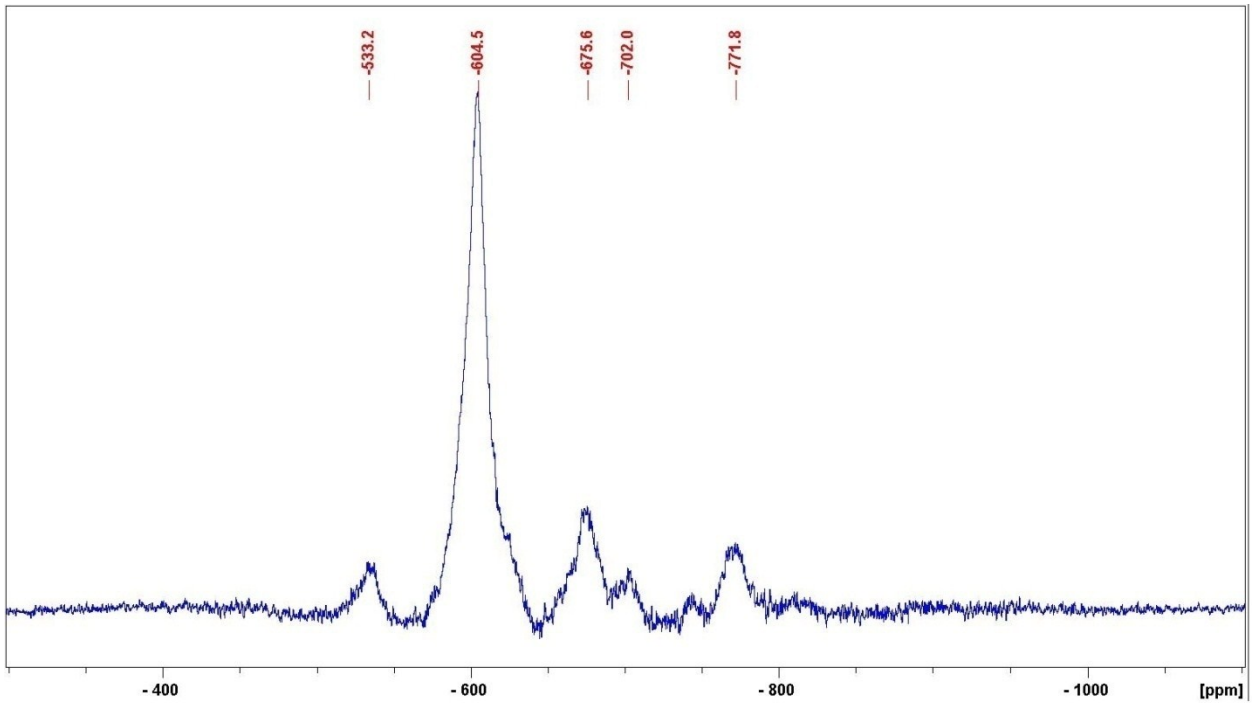


Figure S16: ^{119}Sn MAS 12.5 KHz NMR spectrum of **SnO_2@MSnP**.

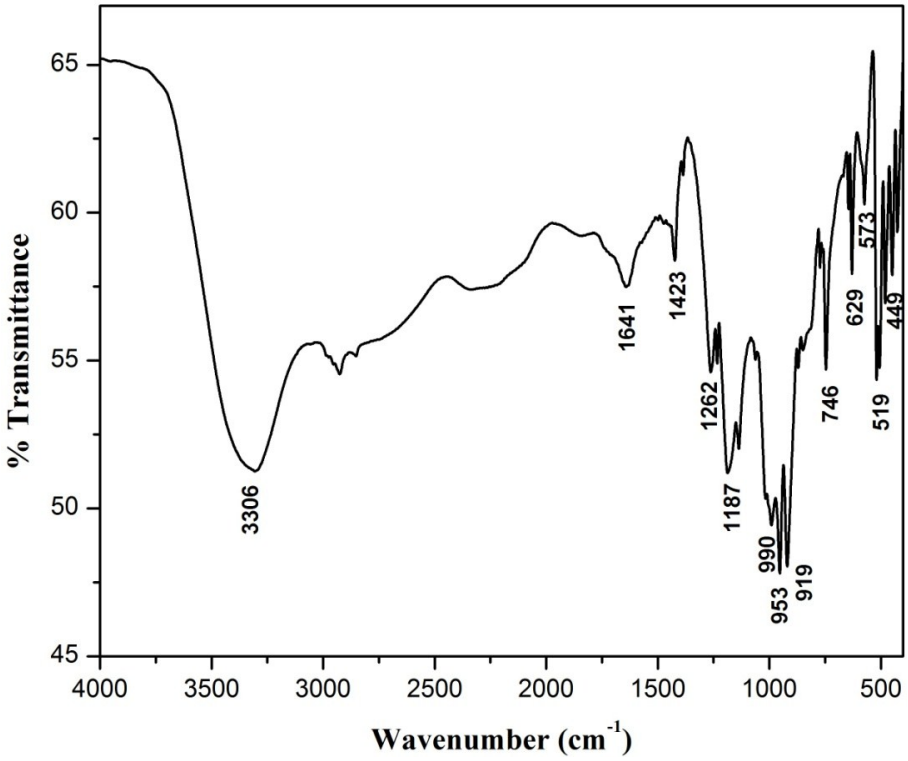


Figure S17: FT-IR spectrum of *Mesityl-1,3,5-tris(methylenephosphonic acid)* as KBr disc.

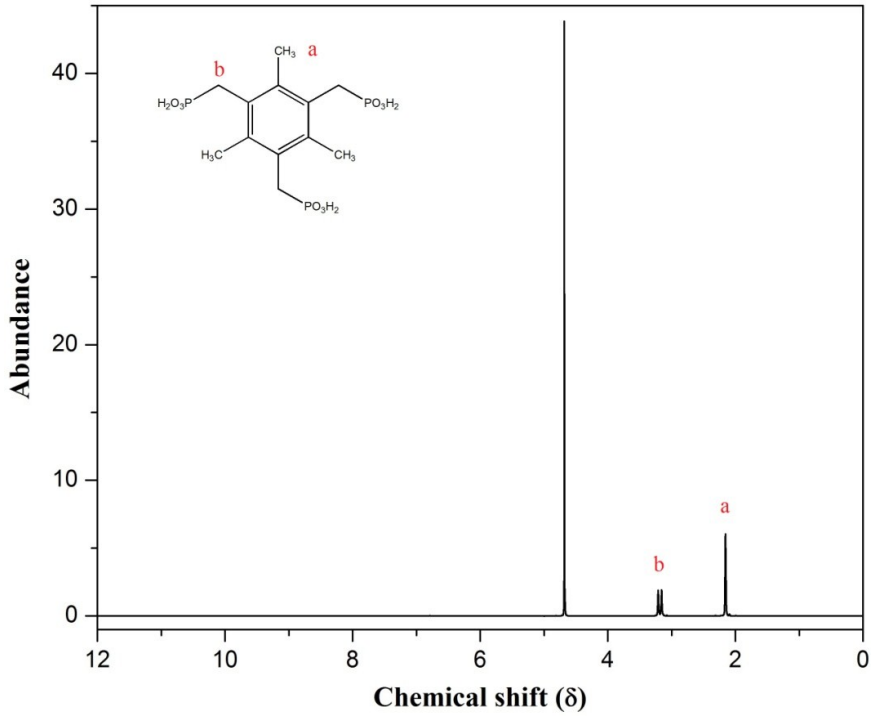


Figure S18: ^{1}H NMR spectra of *Mesityl-1,3,5-tris(methylenephosphonic acid)*.

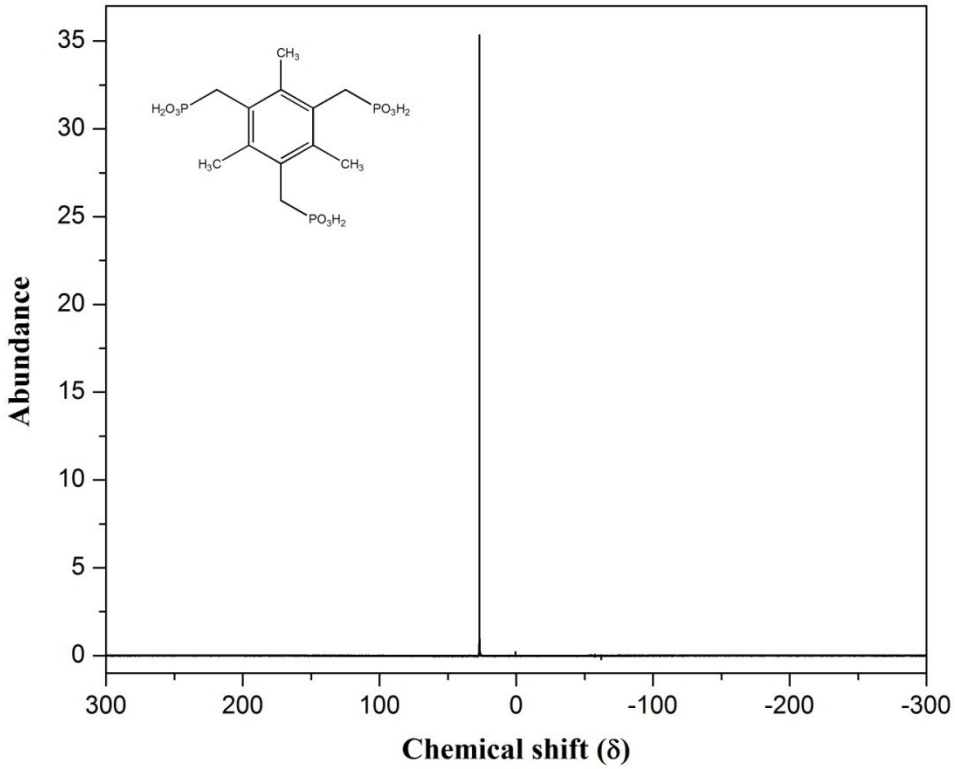


Figure S19: ^{31}P NMR spectra of *Mesityl-1,3,5-tris(methylenephosphonic acid)*.

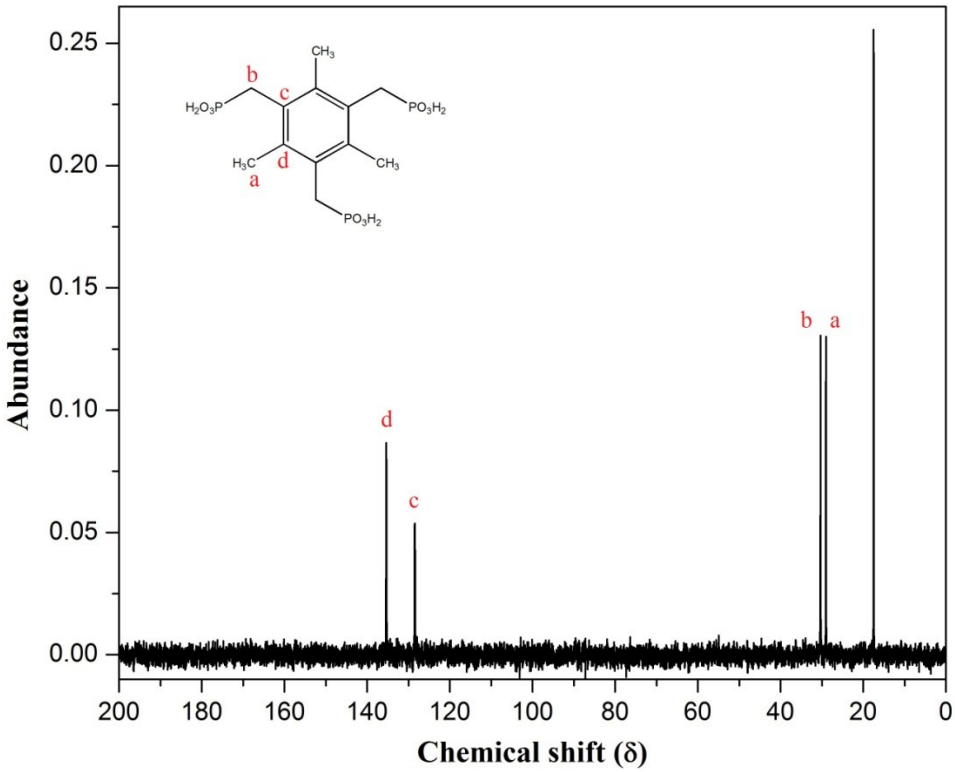


Figure S20: ^{13}C NMR spectra of *Mesityl-1,3,5-tris(methylenephosphonic acid)*.

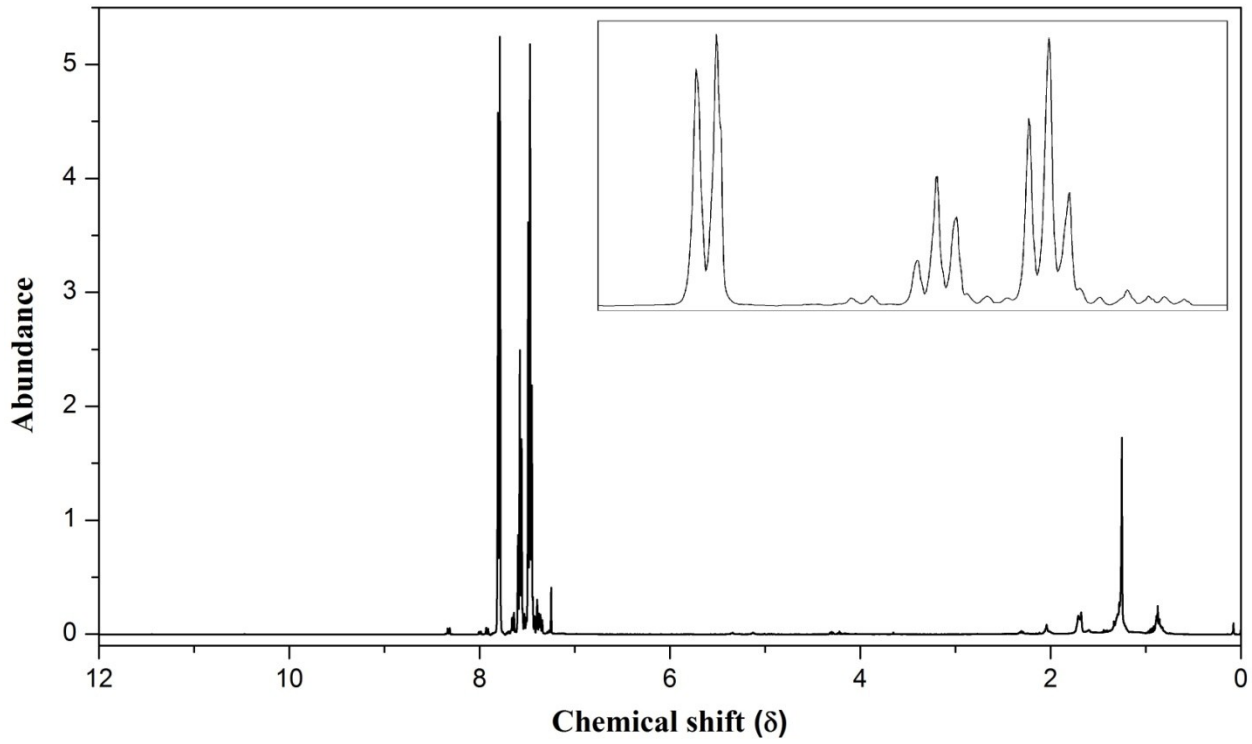


Figure S21:[1]H NMR of product 4.1.b. [1]H NMR ($CDCl_3$, 400MHz, δ ppm): 7.80-7.78 (d, ^3J=7.12, 4H), 7.59-7.55(t, ^3J=7.13, 2H), 7.49-7.45 (t, ^3J=7.20, 4H).

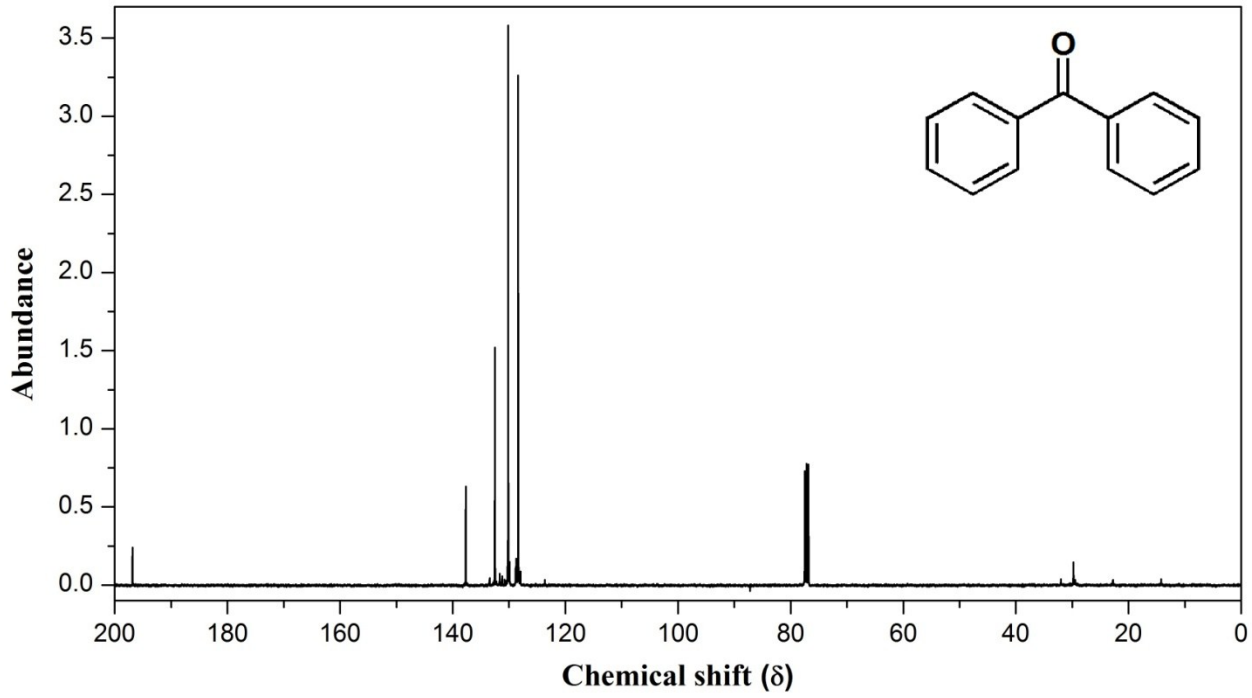


Figure S22:[13]C NMR of 4.1.b. [13]C NMR($CDCl_3$, 100MHz, δ ppm): 196.7, 137.5, 132.4, 130.1, 128.3.

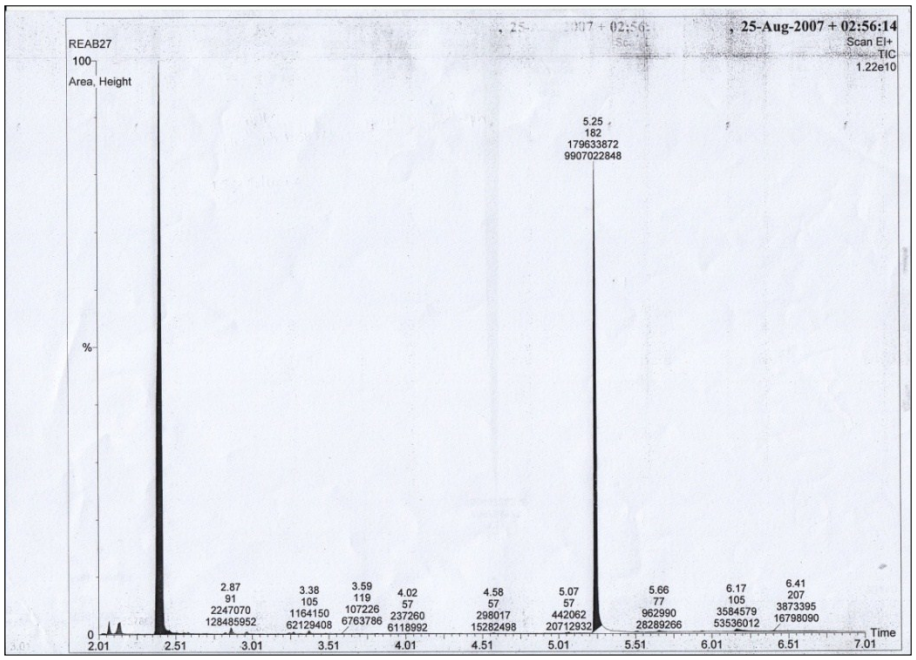


Figure S23: GC spectrum of product 1a from table **1**.

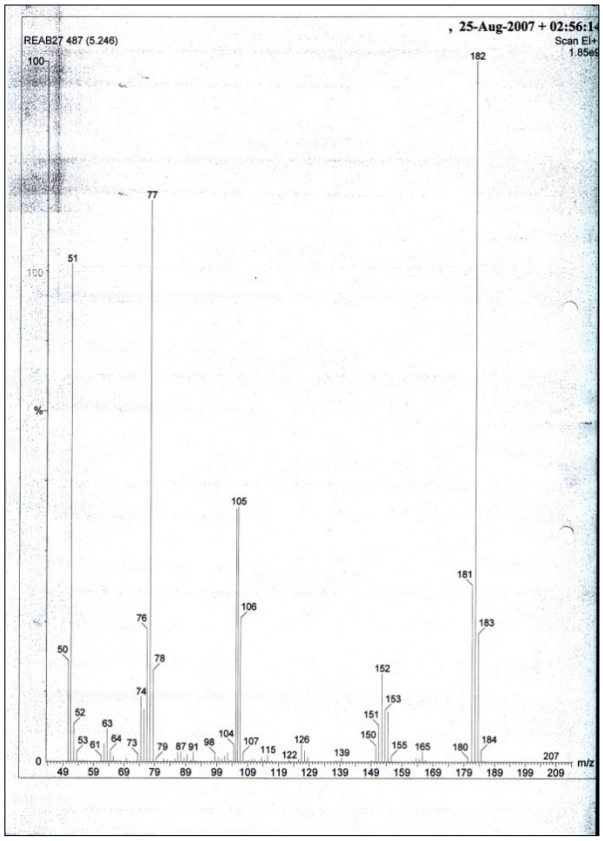


Figure S24: Mass spectrum of product 1a from table **1**.

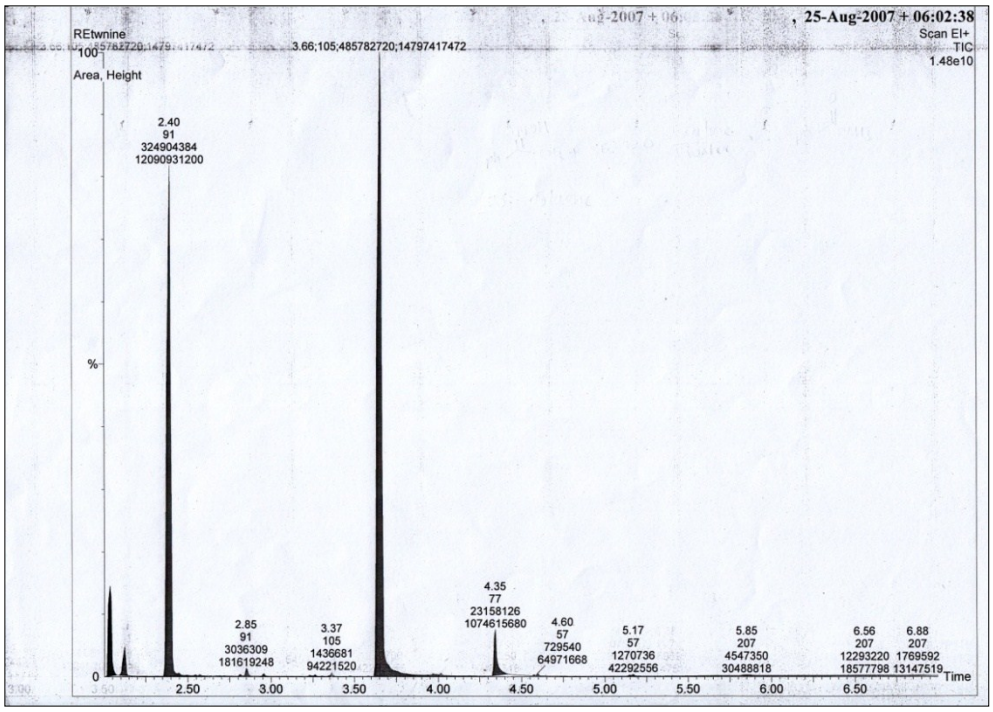


Figure S25: GC spectrum of product 1b from table **1**.

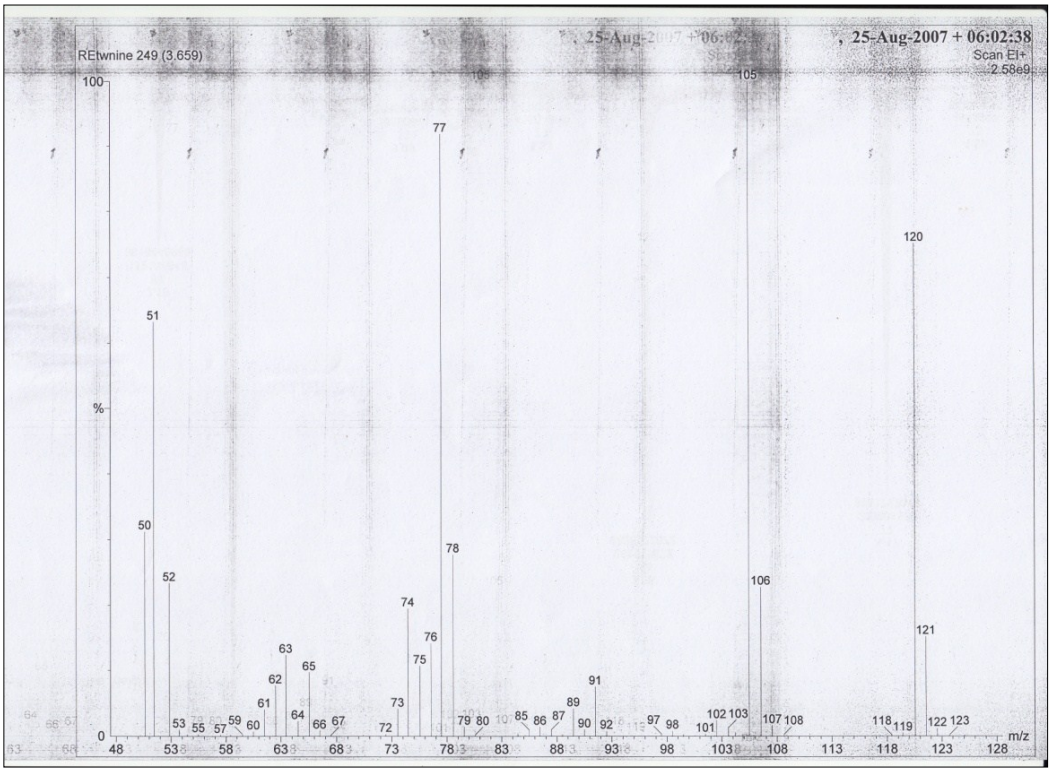


Figure S26: Mass spectrum of product 1b from table **1**.

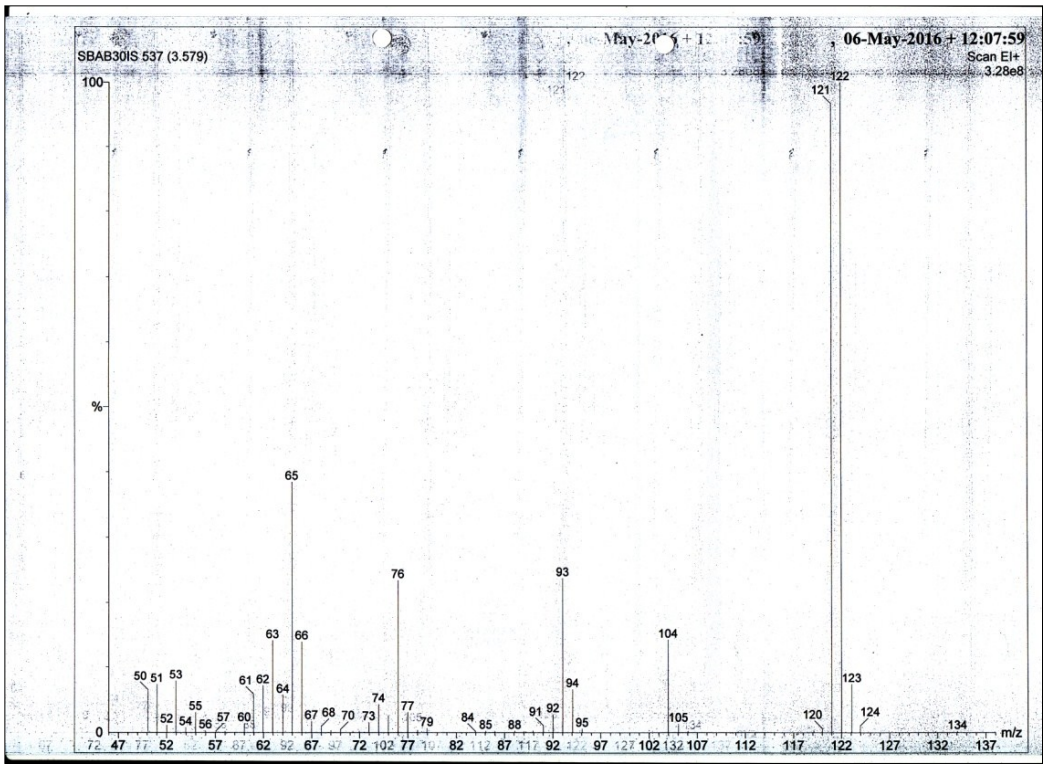


Figure S27: Mass spectrum of product 1c from table **1**.

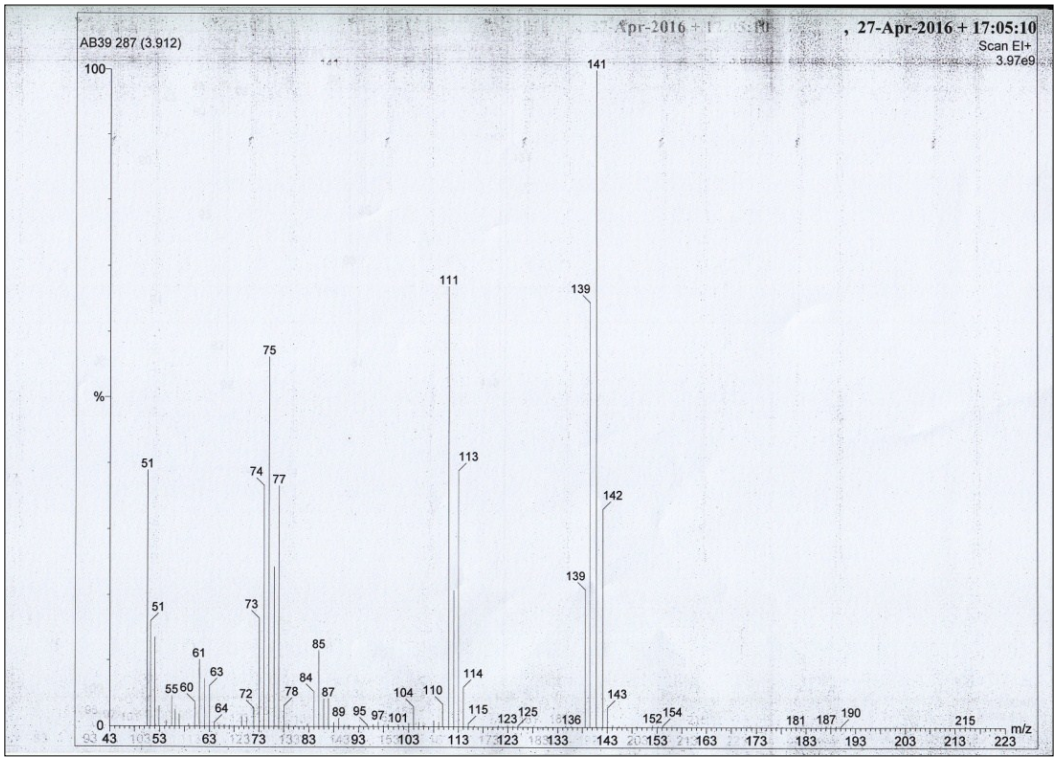


Figure S28: Mass spectrum of product 1e from table **1**.

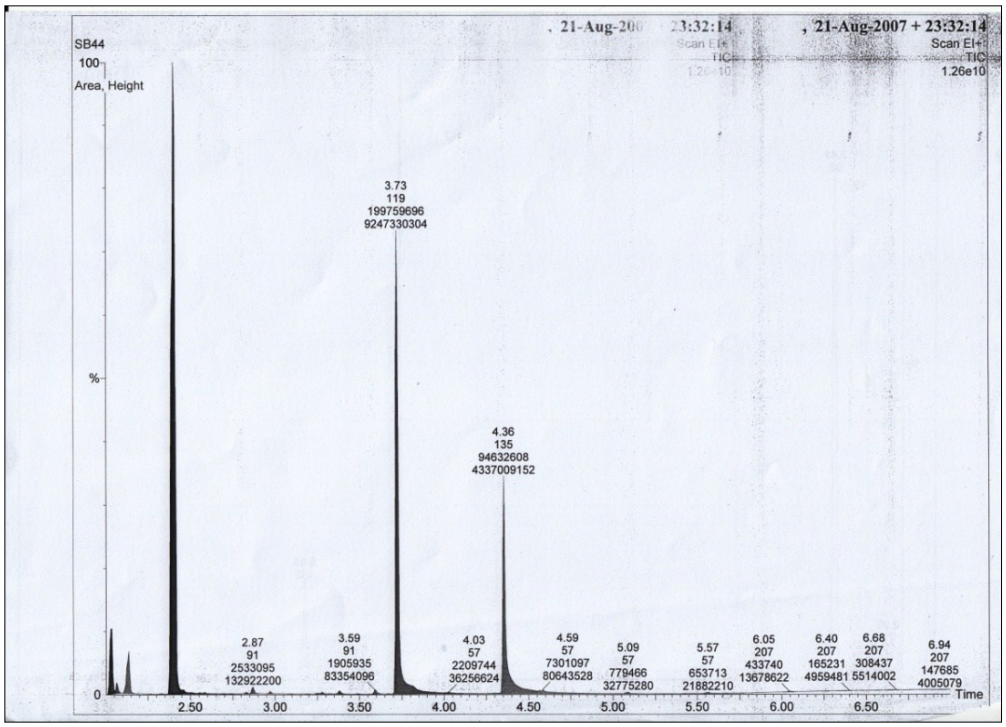


Figure S29: GC spectrum of product 1f from table **1**.

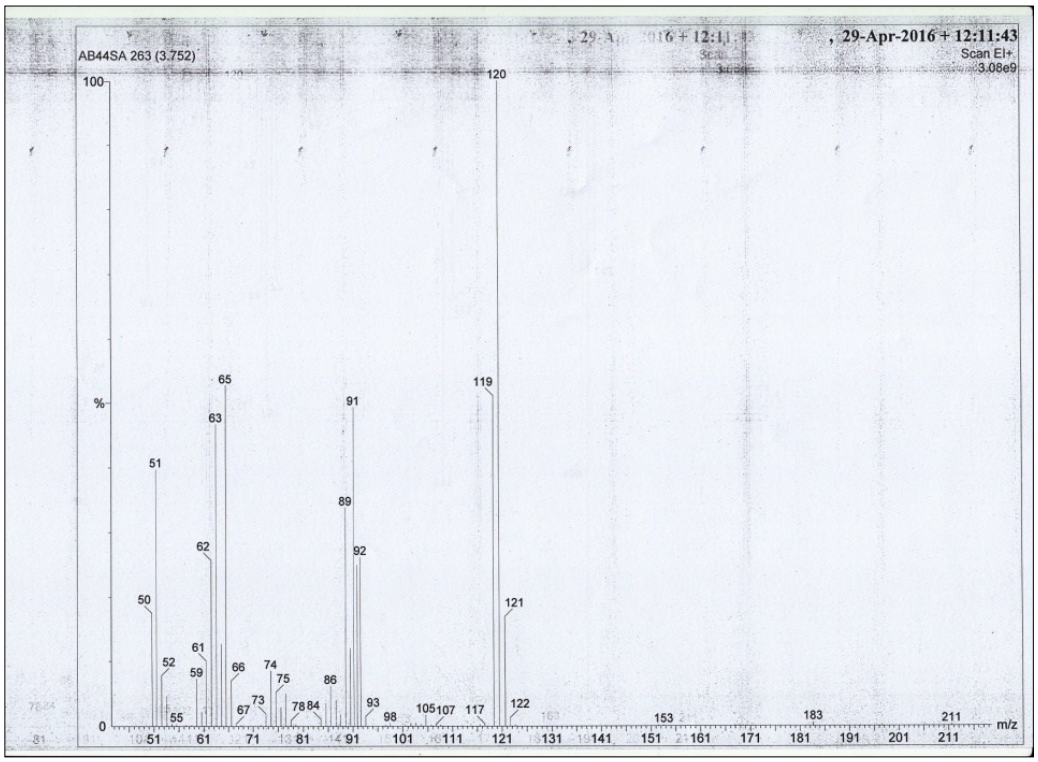


Figure S30: Mass spectrum of product 1f from table **1**.

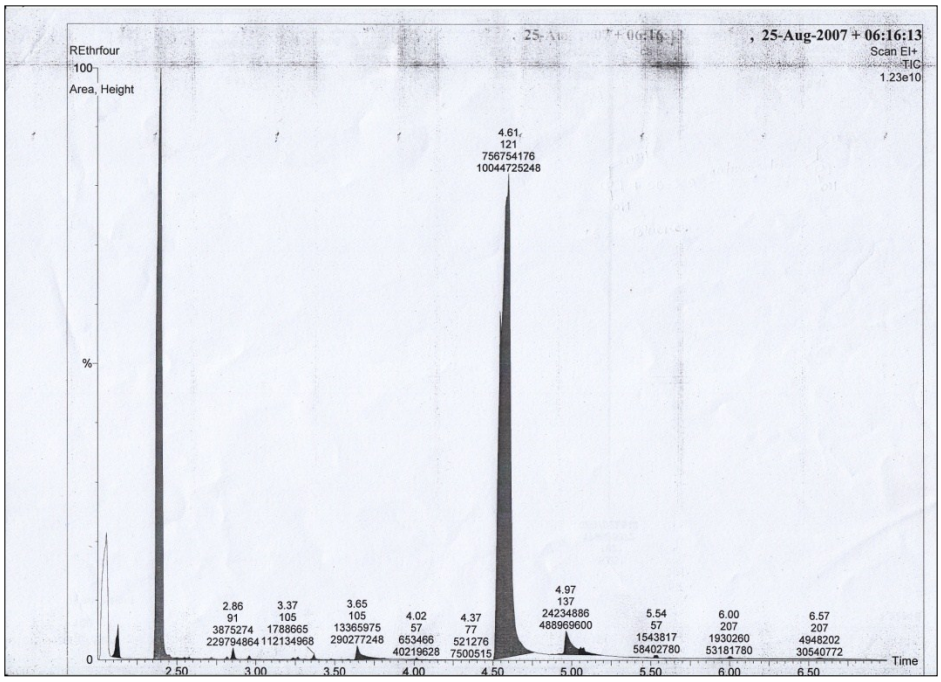


Figure S31: GC spectrum of product 1g from table **1**.

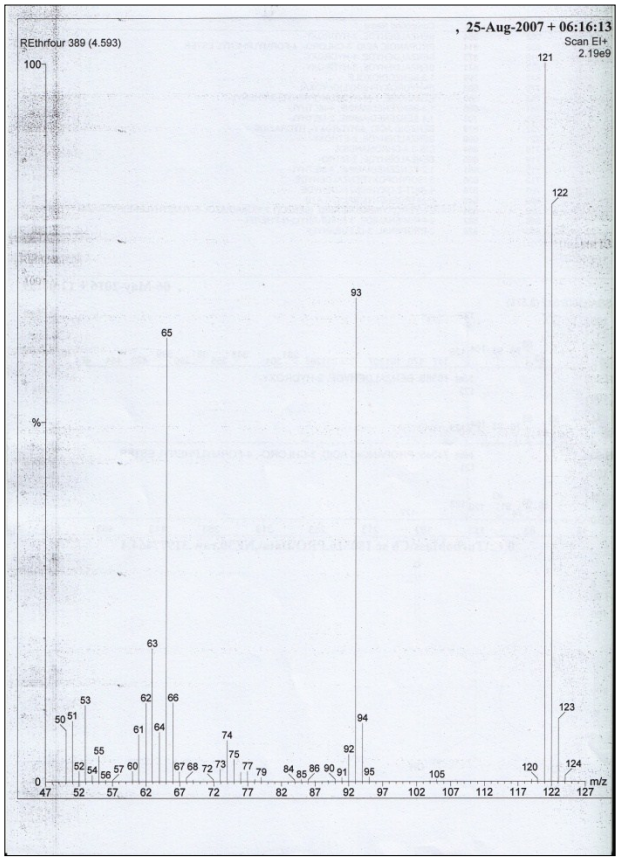


Figure S32: Mass spectrum of product 1g from table **1**.

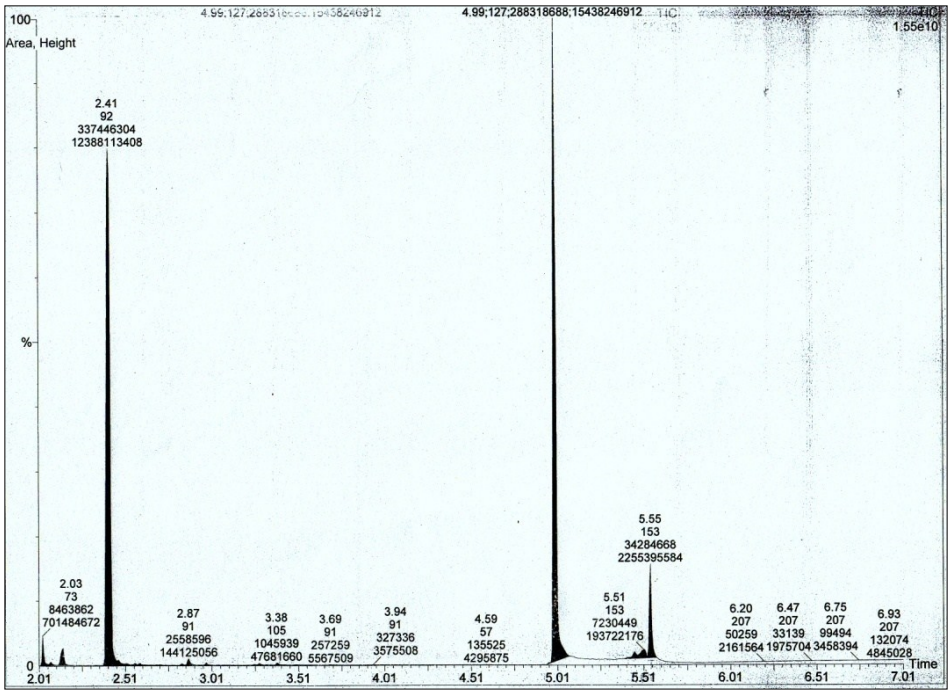


Figure S33: GC spectrum of product 1h from table **1**.

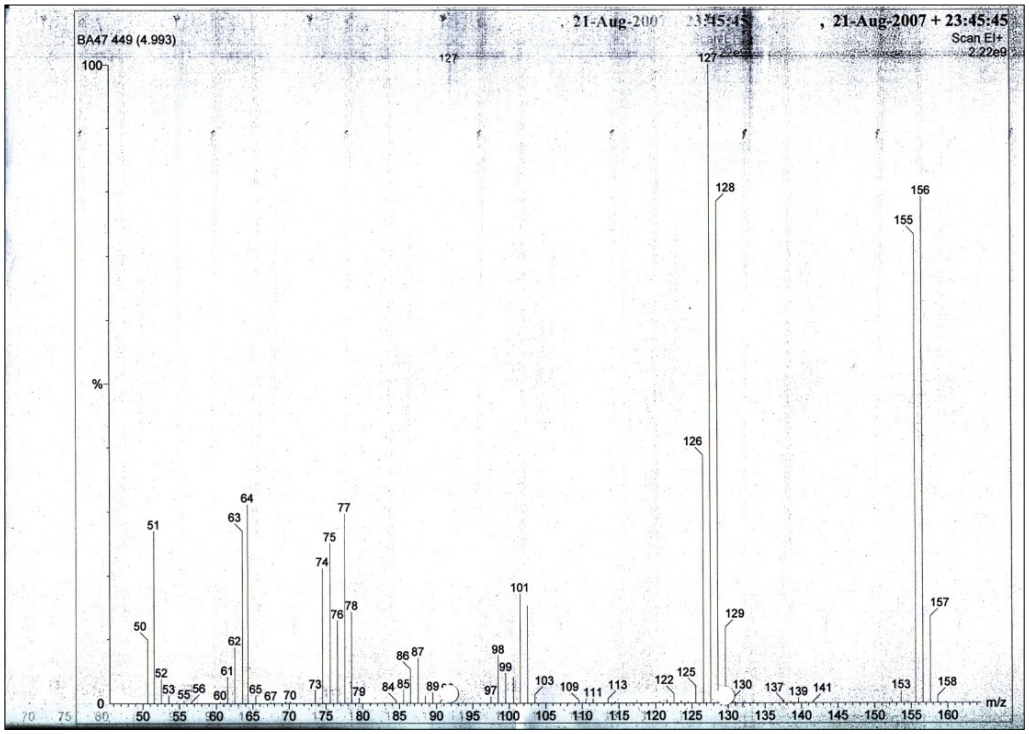


Figure S34: Mass spectrum of product 1h from table **1**.

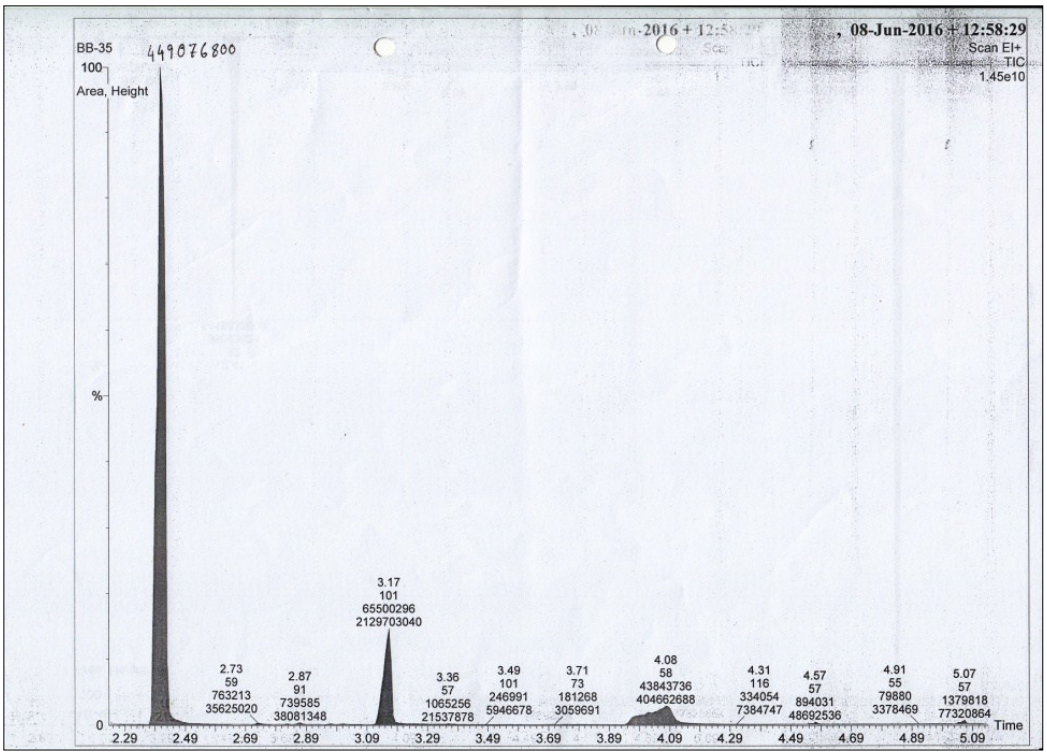


Figure S35: GC spectrum of product 1i from table **1**.

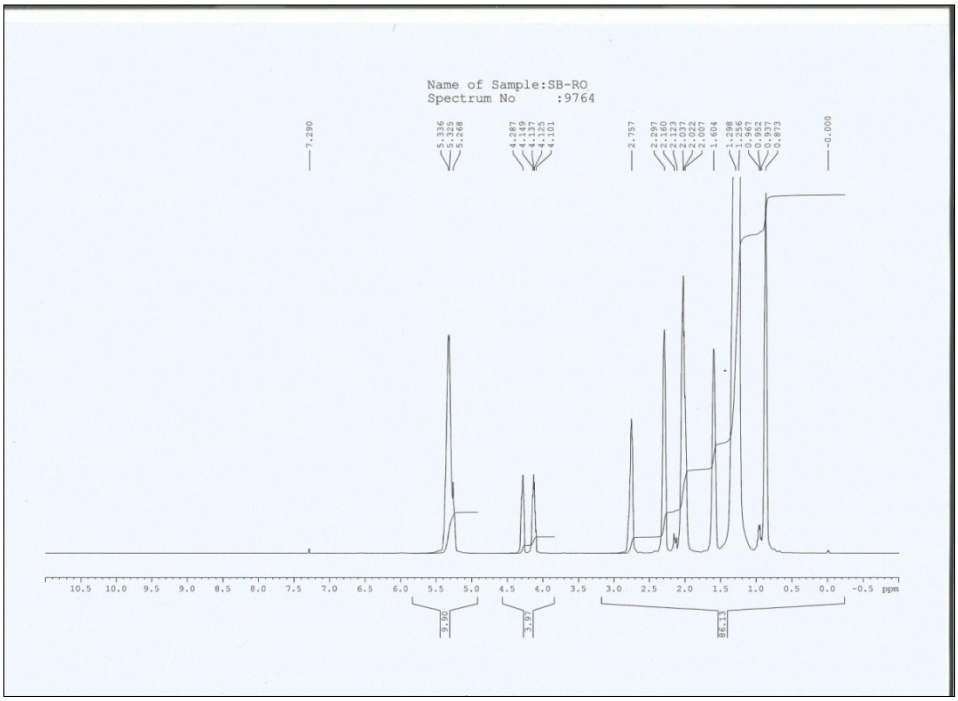


Figure S36: ^{1}H NMR of raw oil for esterification reaction.

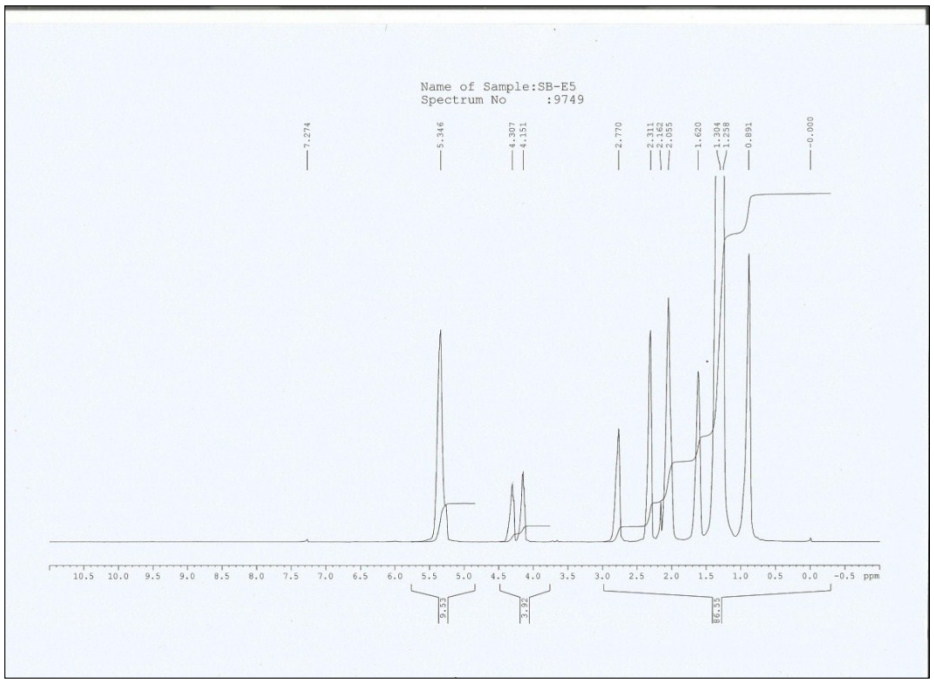


Figure S37: ^{1}H NMR of product after esterification reaction.

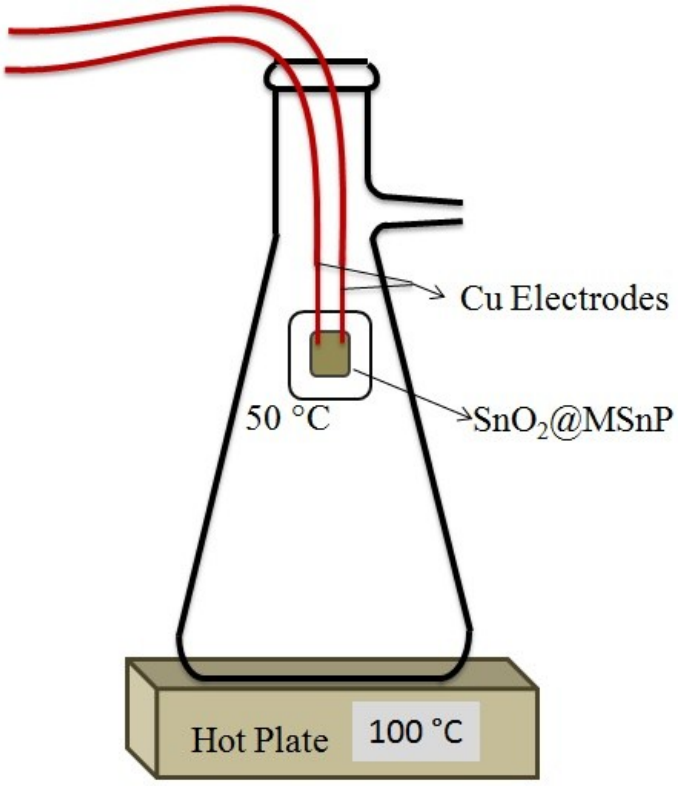


Figure S38: Schematic representation of experimental set up for SnO_2@MSnP gas sensing.

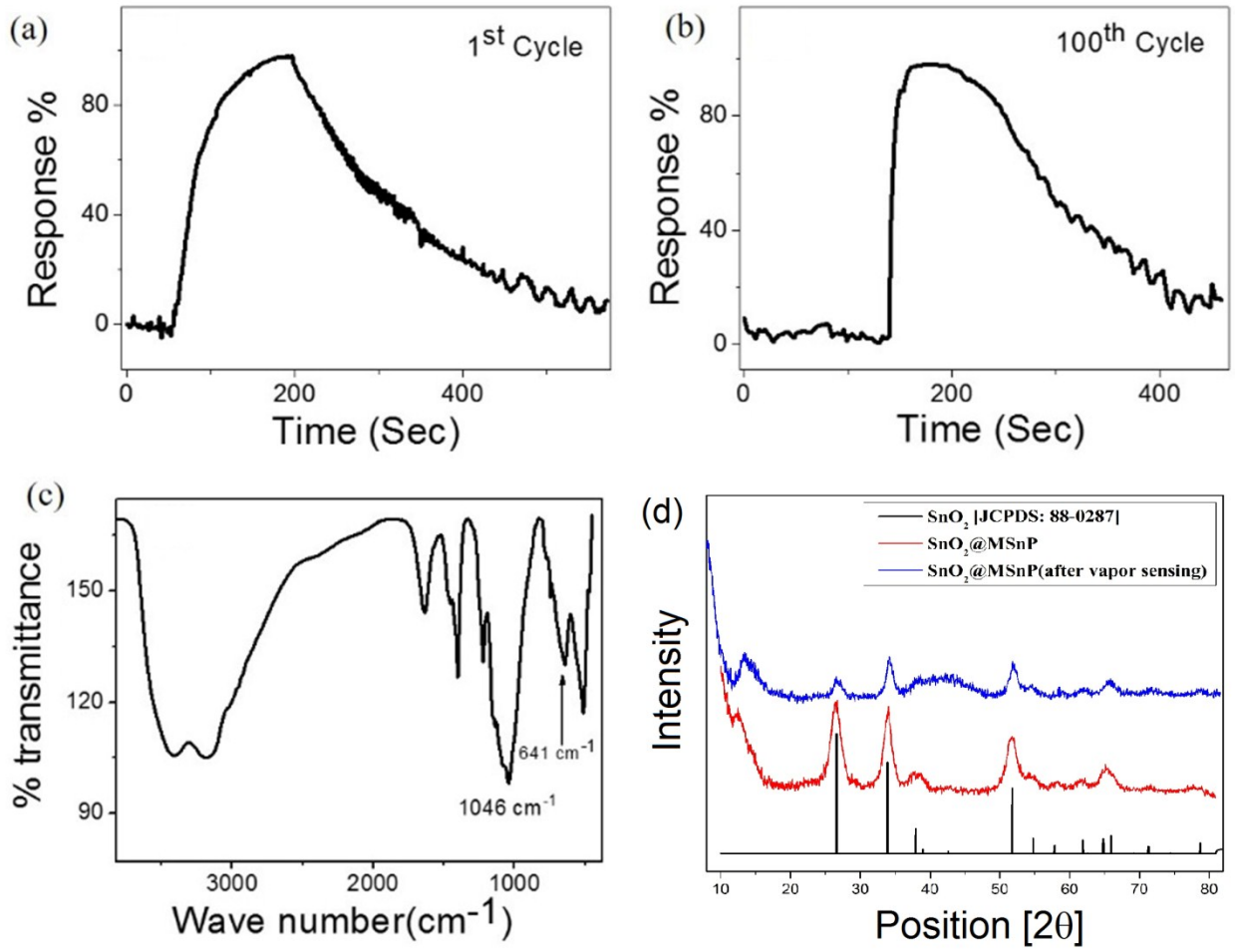


Figure S39: Response curves of SnO_2@MSnP gas sensing device (a) and (b) towards NH_3 gas on 1st and 100th cycle of exposure, (c) IR spectra of SnO_2@MSnP sample recorded after completing gas sensing experiments (d) Powder X-ray diffraction pattern of SnO_2@MSnP sample recorded after completing gas sensing experiments.

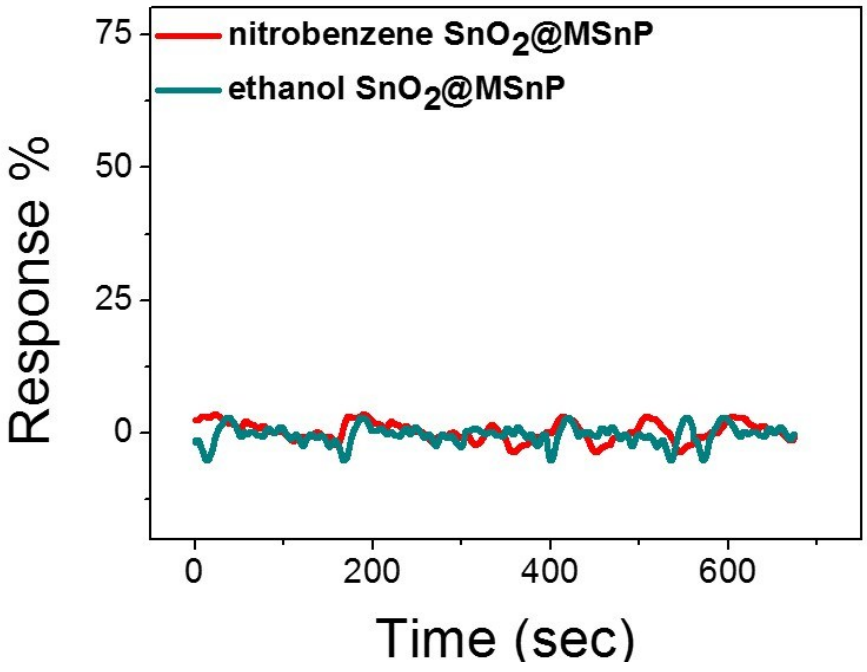


Figure S40: Response curves of SnO_2@MSnP gas sensing device towards nitrobenzene and ethanol vapors.